Microwave and Infrared Spectra of H_2 Containing Complexes with CO, HCN, HCCH

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Hydrogen is one of the most abundant interstellar species. Observation of rotational and vibrational spectra of H_2 containing complexes is of great importance because they are possible candidates for radio-astronomical detection. CO, HCN, HCCH are as isoelectronic molecules of N_2, each with a strong triple bond, but have quite different properties. CO with small dipole is the most commonly used tracer in the interstellar medium. But for higher densities regions, the best probe is using molecules with larger dipole moments, such as HCN. Hence HCN is frequently used to determine the physical and chemical conditions of molecular clouds. In addition HCN is also used as a "faster rotor" doped in helium or hydrogen clusters to study the breakdown the adiabatic following approximation in superfluidity quantum solution. Although acetylene (C_2H_2) has no permanent dipole, the v_3 asymmetric-stretch vibration is Infrared active. In this work, we aimed to obtain accurate and detail theoretical Microwave and Infrared spectra for CO-H_2, HCN-H_2 and HCCH-H_2 complexes, which would provide valuable information for further spectroscopy measurements.

Reliable spectroscopic predictions are based on accurate *ab initio* calculations. Here, five-dimensional ab initio potential energy surfaces (PESs) for CO-H_2, HCN-H_2 and HCCH-H_2 that explicitly incorporates dependence on intra-molecular vibrational stretch coordinate of the CO, HCN, and HCCH monomers have been calculated. Analytic four-dimensional PESs are obtained by least squares fitting vibrationally averaged interaction energies for v = 0 and 1 to the Morse/long-range potential function form with high accuracy. Based on the 4D MLR PESs, the calculated rovibrational energy levels, and Microwave and Infrared spectra for CO, HCN and HCCH with para-H_2 and ortho-H_2 complexes have been predicted, which are in good agreement with those experimental observations.

Reference

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